Computing Nonlinear Thermodynamics in Shape Memory Alloy Wires

Daniel R. Reynolds[1], Petr Kloucek[2]

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[1] **Lawrence Livermore National Lab, reynoldd@llnl.gov**

[2] **Computational & Applied Math, Rice University, kloucek@rice.edu**

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“Smart” Materials and Potential Applications

Active materials exhibit a dramatic, controllable phase transformation

Shape Memory Alloys (SMA):

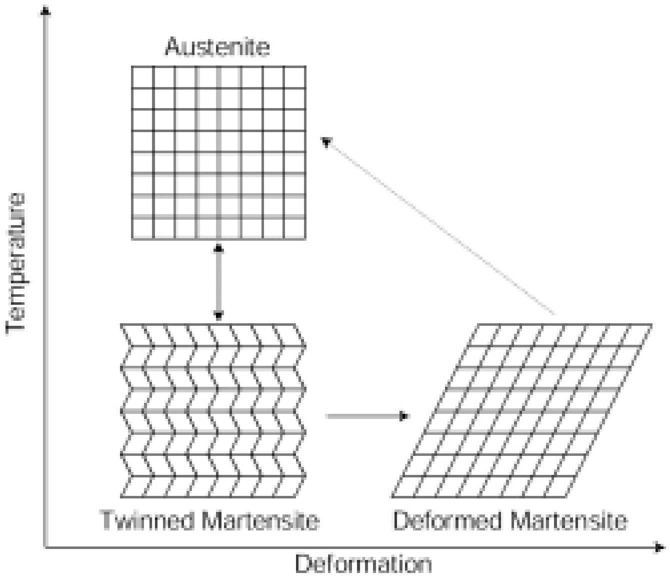
- Thermal $\longrightarrow$ mechanical work
- First discovered in 1932 by A. Olander
- Came to forefront of materials research in 1960s [W.J. Buehler]
- Potential applications include vibration damping, biomedical applications, nanomachinery

SMA Arterial Stent
(from smet.tomsk.ru)

Other active materials with similar phase transformation behavior include Ferromagnets, Piezoelectrics.

First-Order Martensitic Phase Transformation

Materials change elasticity, crystal structure according to temperature and stress:



Shape Memory Effect
(adapted from J. Ryhanen)

Austenite:

- High Symmetry (cubic)
- Single Structure
- Stiff (~ Titanium)

Martensite:

- Low Symmetry (e.g. tetragonal)
- Multiple Structures
- Ductile (~ Soft Pewter)
- Deformations Move Twinning Planes

General Continuum-Thermodynamic Model

The continuum-level thermodynamic description may be given by the following nonlinear system

$$
\begin{aligned}
&\text{(velocity)} && \dot{u} = v, \\
&\text{(momentum)} && \rho_0 \dot{v} = \nabla \cdot (\rho_0 \, \partial_\gamma \Psi + \alpha \nabla v) + \rho_0 \, b, \\
&\text{(energy)} && \rho_0 c_p \dot{\theta} = \left(\rho_0 \, \theta \, \partial^2_{\theta\gamma} \Psi + \dot{\gamma} \, \alpha\right) \cdot \dot{\gamma} + \kappa \, \nabla \cdot (\gamma \, \nabla \theta) + \rho_0 \, r,
\end{aligned}
$$

where $(x,t) \in [0,L] \times R^+$.

The heart of this physical description lies in the construction of the nonlinear free-energy function $\Psi(\gamma,\theta)$.

The Helmholtz Free Energy

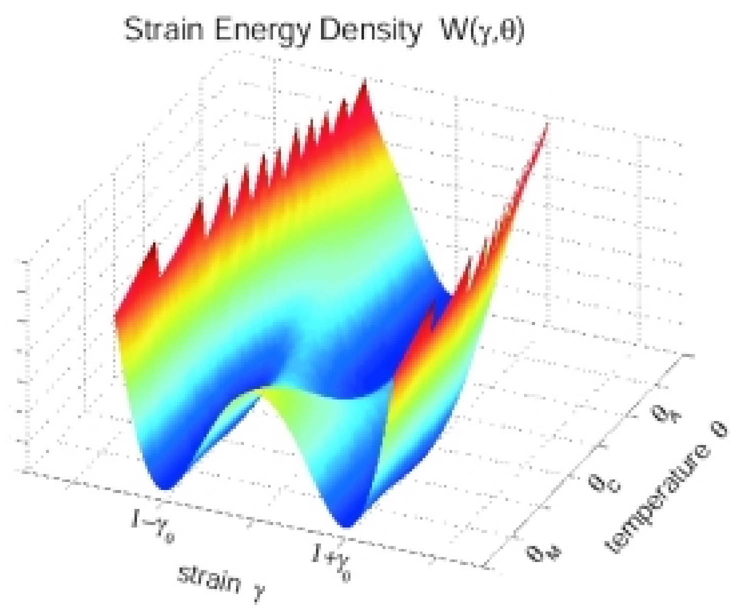
The material physics is described through an expanded form of the Landau-Devonshire potential [Falk 1980; Niezgodka & Sprekels 1988]:

$$\Psi(\gamma,\theta) = W(\gamma,\theta) + c_p\theta(1 - \ln\theta) + D\theta + E$$

$$W(\gamma,\theta) = W_M(\gamma)C_M(\theta) + W_C(\gamma)C_C(\theta) + W_A(\gamma)C_A(\theta)$$

$W_*(\gamma)$ - isothermal elastic profiles

$C_*(\theta)$ - smoothly connect in θ



The strain energy $W(\gamma,\theta)$ (at right) provides the phase transformation (global minima) and satisfies all measurable material constants.

Dealing with the Mathematical Model

Look for weak solutions u,v,θ to the nonlinear system:

$$\int_\Omega \int_{t_n}^{t_{n+1}} (\dot{u} - v)\,\varphi\,dt\,dx = 0,$$

$$\int_\Omega \int_{t_n}^{t_{n+1}} (\rho_0\,\dot{v} - \nabla\cdot(\rho_0 \partial_\gamma \Psi - \alpha\,\nabla v) - \rho_0 b)\,\varphi\,dt\,dx = 0,$$

$$\int_\Omega \int_{t_n}^{t_{n+1}} \Big(\rho_0\,c_p \dot{\theta} - \Big(\rho_0\,\theta\,\partial^2_{\theta\gamma}\Psi - \dot{\gamma}\alpha\Big)\,\dot{\gamma} - \kappa\,\nabla\cdot(\gamma\,\nabla\theta) - \rho_0\,r\Big)\,\varphi\,dt\,dx = 0,$$

Discretizations:

- Spatial discretization uses piecewise affine finite elements
  - due to limited regularity of expected weak solutions
- Temporal discretization uses a two-level, fully-implicit, continuous-time Galerkin method
  - discretely conservative,
  - uniform treatment of space & time.

Dealing with the Model (continued)

The discretized problem results in a fully coupled, finite dimensional, non-convex, root finding problem,

$$g\left(u^{n+1}, v^{n+1}, \theta^{n+1}; u^n, v^n, \theta^n, \alpha\right) = 0.$$

The solver is based on an inexact Newton-Krylov approach:

- Inexactness parameter $\eta_k = \min\left(0.7, \sqrt{||g||_2}\right)$ [Nocedal & Wright]
- Newton system solution uses preconditioned, restarted GMRES.
- Preconditioning uses an incomplete LU factorization of a sparse approximate Jacobian [SPARSKIT2].
- Required globalization combines a backtracking line-search with a viscosity-based continuation method (to be discussed further).

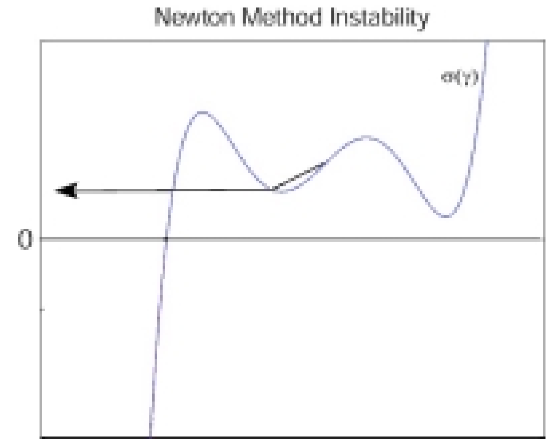
Theoretical Difficulty at the Phase Transition

Desire “small viscosity” solutions:

- Physical experiments observe little or no viscous effects [Seelecke 2002, Seelecke & Muller 2003]
- Linear viscosities unphysical (violate material frame indifference) [Friesecke & Dolzmann 1997, Antman 1998, Antman & Seidman 2003]

Nonconvexity of Ψ requires large α:

- Existence and uniqueness theory only valid for sufficiently large viscosities [Niezgodka & Sprekels 1988, Hoffmann & Showalter 2000]



Small α result in inflection points in the root-finding surface

Viscosity-Based Continuation

Remove instabilities at phase transition through changing viscosity level:

1. Keep a low/zero until beginning of phase transition (tracked using line-search step length)
2. Increase a to compute initial perturbed nonlinear solution
3. Progressively decrease a to pull perturbed solution over energy barrier to low viscosity solution. Attempted the following variations:
   - Begin continuation iterations with previous successful solution
   - Begin with linearly extrapolated solution from two previous successes
   - Perform multiple passes using coarser continuation loop.

Similar to other methods for nonlinear problems:

- Method of Vanishing Viscosity [Hopf 1950, Lax 1954].
- Regularization methods for ill-posed inverse problems.

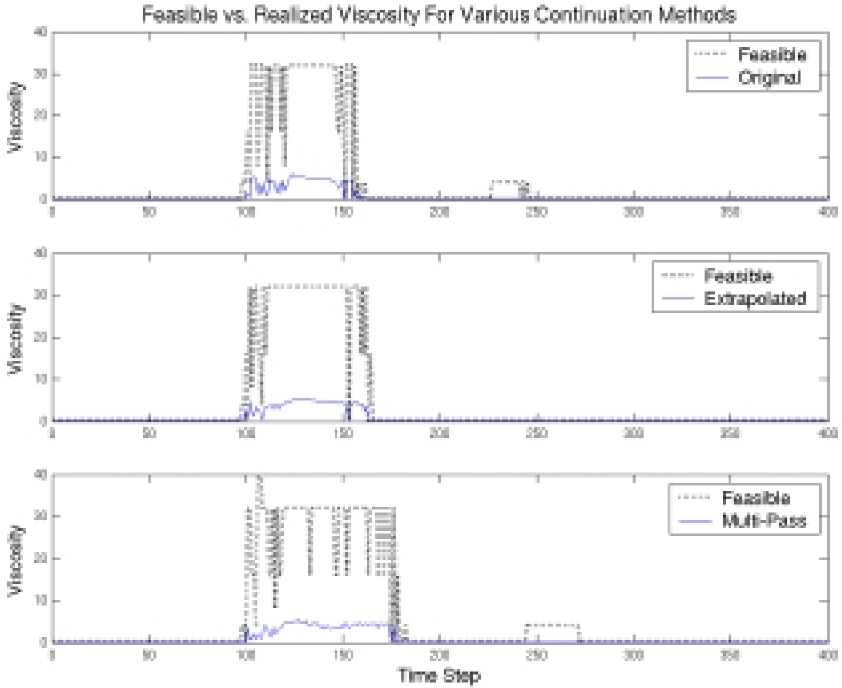
Results of the Viscous Continuation

Much faster than other global methods (e.g. Simulated Annealing):

- “Normal” time steps require (~3 Newton steps)*(~7 GMRES its).
- Phase transitions require ~5 viscosity passes.

Benefits:

- Inflated viscosity only necessary during transition.
- Viscous effects on overall system are measurable and small.
- Continuation dramatically decreases the viscous perturbation required.
- Use of natural variable ensures energy conservation.



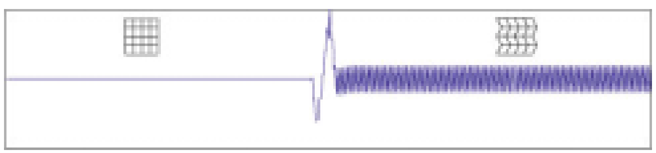
Computations and Visualization

1-D deformation constitutes elongation and contraction from reference state

Displacement is plotted for clarity:

positive = elongation

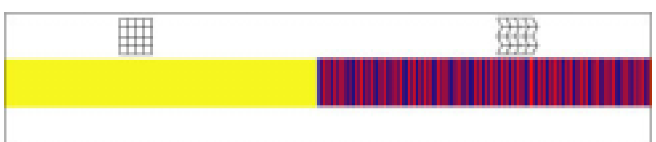
negative = contraction



Phase plots:

yellow = austenite

red/blue = martensite +/-



Constant	Value
L	50 mm
T	2 ms
Δx	5 μm
Δt	1 μs
ρ_0	6.45e+3 kg/m^3
κ	10 W/(K m)
c_p	322 J/(K kg)
E_A	75 GPa
E_M	28 Gpa
θ_M	320 K
θ_M	335 K
θ_A	350 K

NiTi simulation constants

Thermally-Induced Transformations

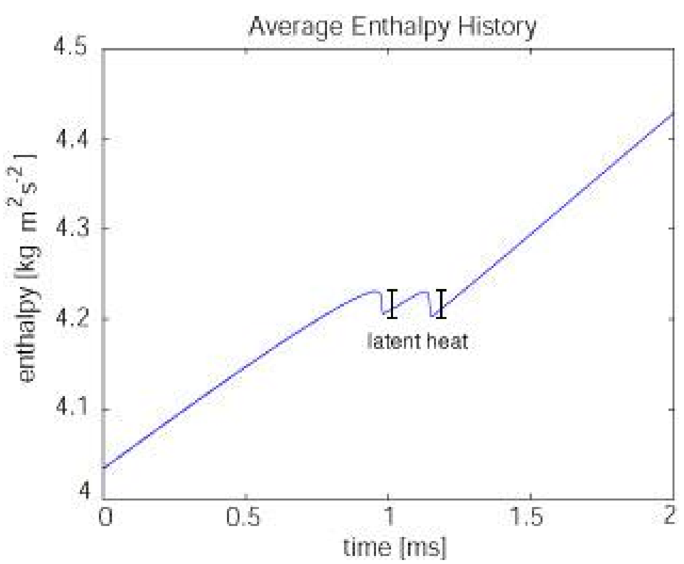
Thermal transformations are induced using a constant heat supply r(x,t):

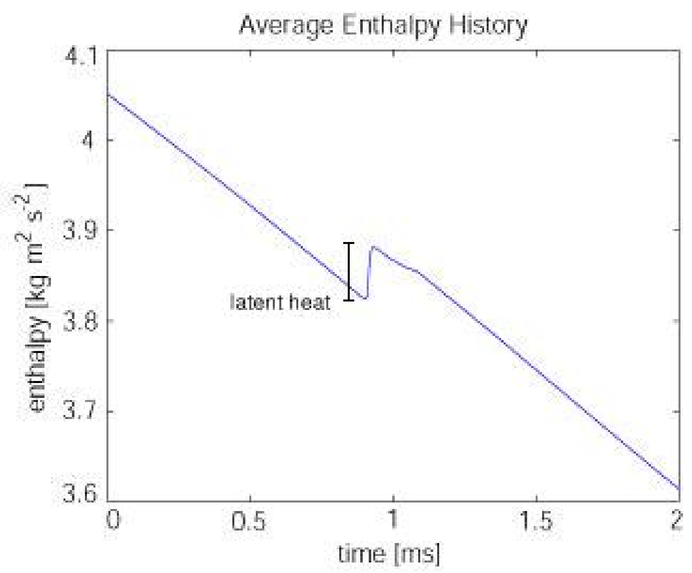
Martensite to Austenite: r = 40 J/s

Austenite to Martensite: r = -40 J/s

Nonlinear latent heat effects are measured by enthalpy jumps.

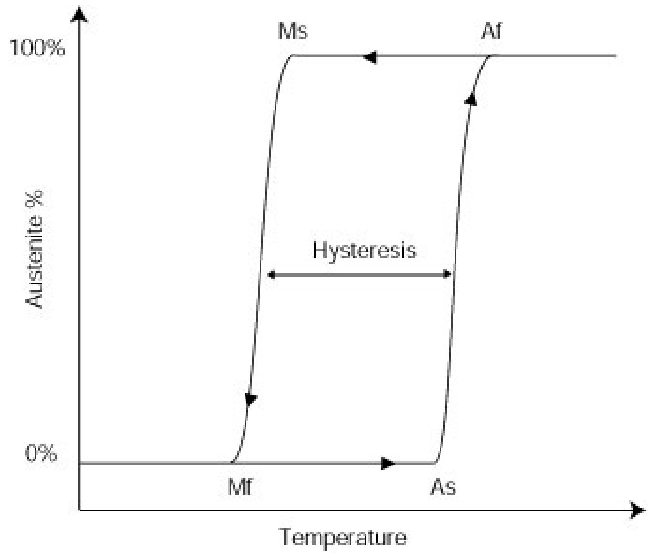
The model successfully predicts these (within a factor of 1.5):



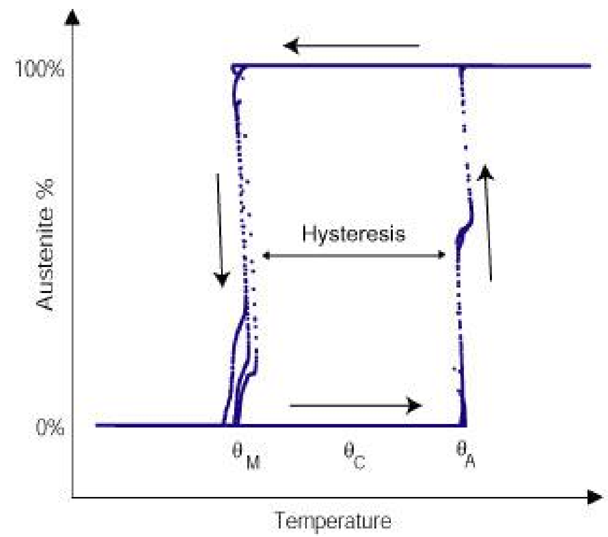


Computed Hysteresis

Hysteresis loop computed using thermally-induced transformations:



Ideal Hysteresis Loop



Computed Hysteresis Loop

- Sharp corners of hysteresis loop likely due to single-crystal model
- Negative tilt due to sharp corners and latent heat of transformation

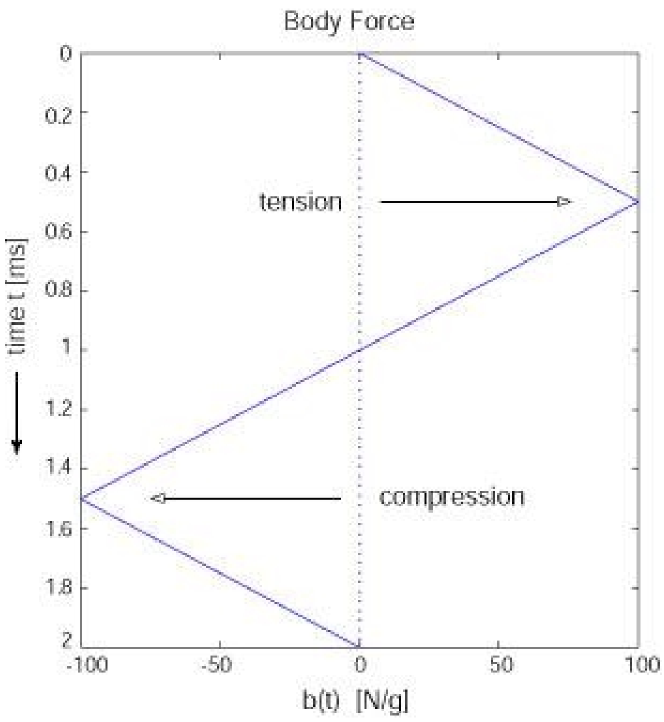
Stress-Induced Transformation

Stress transformations are induced using the body force term b(t):

Simulation Remarks:

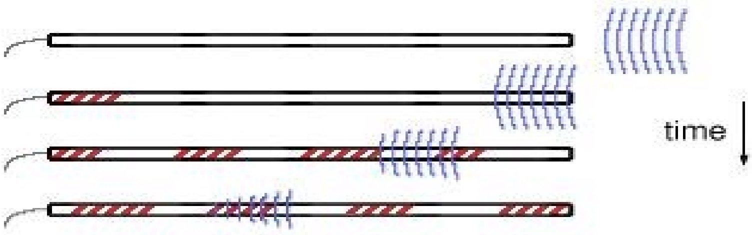
- Begin with relaxed austenite, just below θ_A
- b(t) first extends, then compresses as seen at the right

Simulation Movies

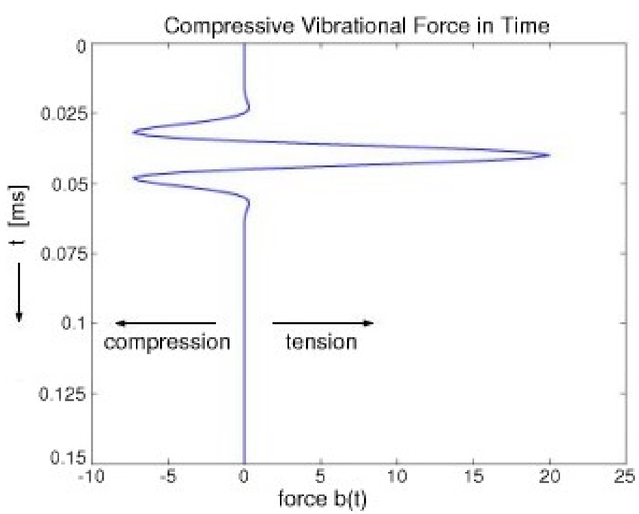


Vibration Experimental Setup

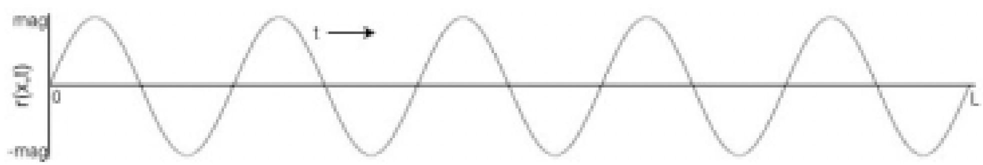
We envision a mechanism for thermally-controlled active damping of vibrations:



To this end, we use a vibrational input force and a localized temperature control:



Localized Temperature Control

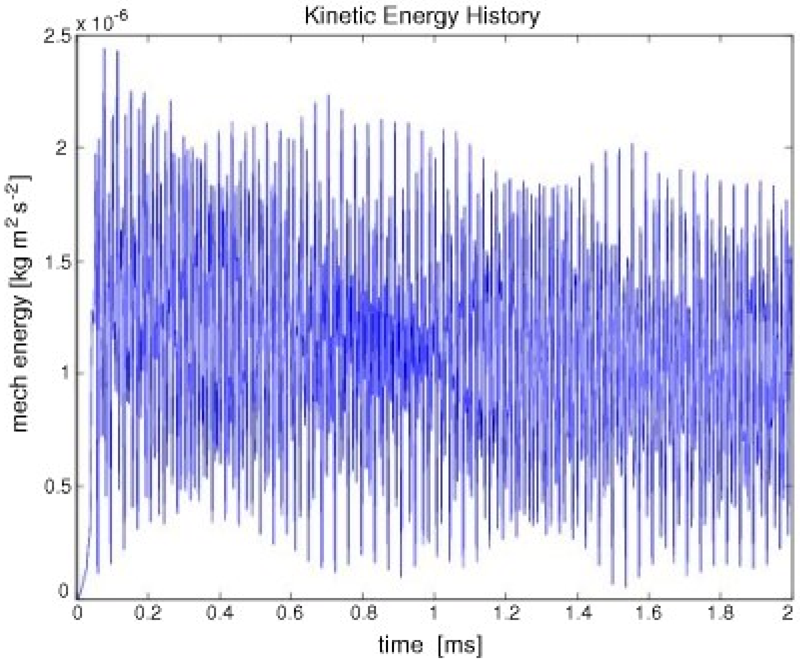


Base Case: No Thermal Control

Simulation Remarks:

- Begin with fully-twinned martensite
- Initial vibrational shock
- Peaks correspond to total vibrational energy
- Continues vibrating with little attenuation

Simulation Movies



Partially-Active Vibration Control

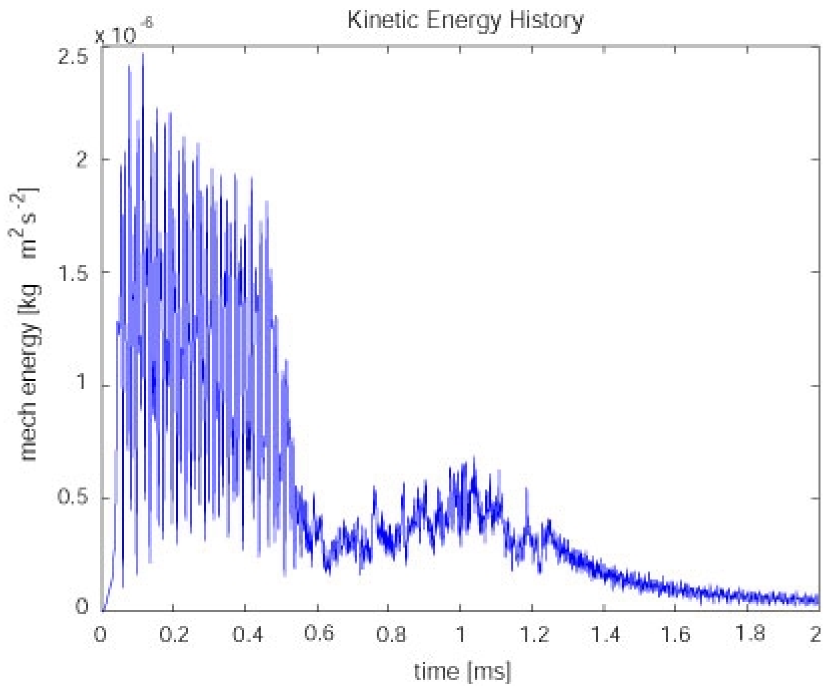
Simulation Remarks:

- Begin with fully-twinned martensite
- Initial vibrational shock
- Localized heating control

$$r(x,t) = 10\sin\left(2\pi\left(\frac{x}{10}+\frac{t}{2}\right)\right) \text{ J/s}$$

- Near-full damping at onset of localized phase transformation

Simulation Movies



Benefits and Limitations of this Approach

Benefits of the modeling and simulation methods include:

- Clean, predictive approach to thermodyanmic modeling of phase transitions
- Successfully describes both phases of SMA, martensitic phase transformation, and material properties
- Iterative solution method based on reliable and scalable components

Limitations include:

- All of the material physics must be encoded in the Helmholtz free energy
- Single-crystal models cannot account for polycrystalline structure and material defects found in production alloys
- One space dimension loses some physics of the full material
- ILU preconditioner does not scale with problem size (for future higher-dimensional modeling)

Directions for Future Research

- Consider alternative continuation methods
  - Viscous continuation in spatially localized regions
  - Adaptive time-stepping around moments of transition
- Construct preconditioner based on standard linearized SMA models
- Extend modeling system to thin films (currently underway) and solids
- Examine optimal thermal controls for active damping with SMA
- Examine modeling approaches based on a stochastic description of the free energy (polycrystalline materials, defects)

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Viscosity-Based Continuation

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